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SUMMARY

In the present work we show the analysis of an approximate solution for the connected kinetic differential equations of a defect involving processes of untrapping, retrapping and recombination annihilation, using the Dulac–Poincaré theorem.

I. INTRODUCTION

The kinetic decay and growth of defects in crystals and amorphous materials have been subject of many studies through luminescence, EPR and optical absorption techniques [1,2]. Our previous studies on the kinetics of defects in crystals and amorphous materials suggested that kinetics of point defects can be described in terms of concentrations of defects coupled through differential equations [3–13]. The general form of the kinetic equation for the i–th concentration defects, y_i, is:

$$\dot{y}_i = f_i(t, y_1, \ldots, y_i, \ldots, y_k) \quad , \qquad (1)$$

where $y_1, \ldots, y_i, \ldots, y_k$ are the concentrations of defects and f_i is a non–linear function.

The thermal dependence of the parameters in f_i were analysed in terms of free–particles distribution of speeds [14,15] and the non–linear stability analysis applied to the kinetic differential equations showed that these equations have stable solutions [16].

The method of Runge–Kutta [17] used to solve the differential equations became unstable for large values of parameters and small number of steps. Then, for good convergence, many times the time interval must be divided in large number of steps, increasing the time of computation. Then, for a fast analysis of the kinetics, an approximate solution which reproduce the essential behavior of kinetics is wellcome.

In the present report we show the analysis of an approximate solution for the kinetic differential equations (1), using the Dulac–Poincaré theorem [18].

II. THE APPROXIMATE SOLUTION

The kinetic decay of a defect, in the simplest case, involves processes of untrapping of trapped particles, retrapping of free–particles and recombination annihilation of these free particles with trapped antiparticles. Let be y_1 concentration of trapped particles; y_3 concentration of free particles; y_4 concentration of free traps of particles; y_2 concentration of antiparticles and y_5 concentration of free traps of antiparticles. The kinetic equations are:

$$\frac{dy_1}{dt} = -\alpha y_1 + \gamma y_3 y_4 \quad , \qquad (2a)$$

$$\frac{dy_3}{dt} = \alpha y_1 - \gamma y_3 y_4 - \beta y_3 y_5 \quad , \qquad (2b)$$

$$\frac{dy_4}{dt} = \alpha y_1 - \gamma y_3 y_4 \quad , \qquad (2c)$$

$$\frac{dy_2}{dt} = -\beta y_3 y_5 \quad , \qquad (2d)$$

$$\frac{dy_5}{dt} = \beta y_3 y_5 \quad . \qquad (2e)$$

If the concentration of traps of particles is F_0 and of traps of antiparticles is E_0, then

$$F_0 = y_1 + y_4 \quad , \qquad (3a)$$

$$E_0 = y_2 + y_5 \quad . \qquad (3b)$$

The charge conservation gives

$$y_2 = y_1 + y_3 \quad . \tag{4}$$

From equations (3) and (4) we disconnect equations (2). The resultant system of connected equations is:

$$\frac{dy_1}{dt} = -\alpha y_1 + \gamma \{F_0 - y_1\} y_3 \quad , \tag{5a}$$

$$\frac{dy_3}{dt} = \alpha y_1 - \gamma \{F_0 - y_1\} y_3 - \beta \{y_1 + y_3\} y_3 \quad . \tag{5b}$$

The kinetic equations (5) form an autonomous dynamic system: a set of first order differential equations with two variables, y_1 and y_3, whose right hand of the equations are not explicity time dependet.

For the analysis of an approximate solution let us rewrite equations (5) in the form:

$$\dot{y}_1 = -a\, y_1 + c\, y_2 - \gamma y_1 y_2 + \gamma y_1^2 \quad , \tag{6a}$$

$$\dot{y}_2 = \beta y_1 y_2 - \beta y_2^2 \quad , \tag{6b}$$

where $a = \alpha + \gamma F_0$ and $c = \gamma F_0$.

The equations (6) can be rewriten as a sum of a linear term and a non–linear term:

$$\frac{d}{dt}\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = A \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} \gamma (y_1^2 - y_1 y_2) \\ \beta (y_1 y_2 - y_2^2) \end{bmatrix} \quad , \tag{7}$$

where the first term is the linear term and the second term the non–linear term, and with

$$\mathbf{A} = \begin{bmatrix} -a & c \\ 0 & 0 \end{bmatrix} \quad .$$

The equation (6) can be best analysed in a system of coordinates in which the linear term is diagonalized through the transformation

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{T} \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} \quad , \tag{8}$$

where $\mathbf{T} = [v^1, v^2]$. The column matrices v^1 and v^2 are the eigenvalues of the secular equation:

$$[\mathbf{A} - \lambda\, \mathbf{I}]\, v = 0 \quad . \tag{9}$$

Solving this equation we obtain, $\lambda_1 = -a$, $\lambda_2 = 0$ and

$$v^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad , \quad v^2 = \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} \quad ;$$

where $\xi_2 = c/\sqrt{a^2+c^2}$ and $\xi_2 = a/\sqrt{a^2+c^2}$. Then

$$y_1 = \eta_1 + \xi_1 \eta_2 \quad . \tag{10a}$$

$$y_2 = \xi_2 \eta_2 \quad . \tag{10b}$$

The transformation $\mathbf{T}$ changes equations (7) to:

$$\dot{\eta}_1 = -a\,\eta_1 + a_{11}\,\eta_1^2 + a_{22}\,\eta_2^2 + a_{12}\,\eta_1\,\eta_2 \quad , \tag{11a}$$

$$\dot{\eta}_2 = b_{22}\,\eta_2^2 + b_{12}\,\eta_1\,\eta_2 \quad , \tag{11b}$$

where $a_{11} = \gamma$, $a_{22} = (\gamma - \beta)\,\xi_1(\xi_1 - \xi_2)$, $a_{12} = (2\gamma - \beta)\xi_1 - \xi_2$, $b_{22} = \beta\,(\xi_1 - \xi_2)$ and $b_{12} = \beta$.

According to the Dulac–Poincaré theorem we can write the solution of equations (11) as

$$\eta_1 = \sum_{n=0}^{\infty} \zeta_1^n \sum_{m=0}^{\infty} X_{n,m}^{(i)}\,\zeta_2^m \quad , \tag{12}$$

where

$$\dot{\zeta}_1 = \zeta_1 \sum_{n=0}^{\infty} g_n^{(1)}\,\zeta_2^n \quad ,$$

$$\dot{\zeta}_2 = \sum_{n=0}^{\infty} g_n^{(2)}\,\zeta_2^n \quad .$$

From equations (13) we obtain

$$\int_0^t \frac{d\,\zeta_2}{\sum_{n=0}^{\infty} g_n^{(2)}\,\zeta_2^n} = t \quad , \tag{13a}$$

$$\ln\left[\zeta_1(t)/\zeta_1(0)\right] = \int_0^t \left[\sum_{n=0}^{\infty} g_n^{(1)}\,\zeta_2^n(t')\right] dt' \quad . \tag{13b}$$

For second order expansion we have:

$g_2^{(2)} = b_{22}$, $g_1^{(1)} = a_{12}$, $X_{02}^{(1)} = a_{22}/a$, $X_{20}^{(1)} = -a_{11}/a$, $X_{11}^{(2)} = -b_{12}/a$ and $X_{20}^{(2)} = -b_{11}/2a = 0$. Then

$$\zeta_2 = \frac{1}{D + rt} \quad , \tag{14a}$$

$$\zeta_1 = F\,e^{-at + \Gamma \ln \zeta_2} \quad , \tag{14b}$$

where D and F are arbitrary parameters,

$$r = \alpha\beta/\sqrt{a^2 + c^2} \quad ,$$

$$\Gamma = \frac{\alpha - (2\gamma - \beta - 1)c}{\alpha\beta} \quad .$$

From equations (12) and (14) we obtain

$$\eta_1 = \zeta_1 + \frac{a_{22}}{a}\zeta_2^2 - \frac{a_{11}}{a}\zeta_1^2 \quad , \tag{15a}$$

$$\eta_2 = \zeta_2 - \frac{b_{12}}{a}\zeta_1\,\zeta_2 \quad . \tag{15b}$$

III. RESULTS

From equations (10), (14) and (15) we can evaluate y_1 and y_2 using initial conditions $y_1(0)$ and $y_2(0)$ to evaluate D and F. The application of these conditions leave to the equations:

$$y_1^0 = \eta_1(D,F;0) + \xi_1\, \eta_2(D,F;0) = y_1(D,F;0) \quad , \tag{16a}$$

$$y_2^0 = \xi_2\, \eta_2(D,F;0) = y_2(D,F;0) \quad ; \tag{16b}$$

where

$$\eta_1(D,F;0) = \frac{F}{D^\Gamma} + \frac{a_{22}}{a}\frac{1}{D^2} - \frac{\gamma}{a}\left[\frac{F}{D^\Gamma}\right]^2 ,$$

$$\eta_2(D,F;0) = \frac{1}{D} - \frac{\beta}{a}\frac{\Gamma}{D^{\Gamma+1}} \quad ,$$

$$\frac{a_{22}}{a} = -\frac{c\ \alpha\ (\gamma - \beta)}{a\sqrt{a^2 + c^2}} \quad .$$

We calculate D and F using the method of Newton–Raphson. First we define the functions:

$$F_1(D,F) = y_1(D,F;O) - y_1^0 \quad , \tag{17a}$$

$$F_2(D,F) = y_2(D,F;O) - y_2^0 \quad . \tag{17b}$$

where y_1^0 and y_2^0 are the initial conditions. These functions are expanded to second order giving:

$$\begin{bmatrix} F_1(D_n,F_n) \\ F_2(D_n,F_n) \end{bmatrix} + \begin{bmatrix} \frac{\partial F_1}{\partial D_n} & \frac{\partial F_1}{\partial F_n} \\ \frac{\partial F_2}{\partial D_n} & \frac{\partial F_2}{\partial F_n} \end{bmatrix} \begin{bmatrix} D_{n+1} - D_n \\ F_{n+1} - F_n \end{bmatrix} = 0 \tag{18}$$

$$\begin{bmatrix} D_{n+1} \\ F_{n+1} \end{bmatrix} = \begin{bmatrix} D_n \\ F_n \end{bmatrix} - \begin{bmatrix} \frac{\partial y_1}{\partial D_n} & \frac{\partial y_1}{\partial F_n} \\ \frac{\partial y_2}{\partial D_n} & \frac{\partial y_2}{\partial F_n} \end{bmatrix}^{-1} \begin{bmatrix} y_1(D_n,F_n;0) - y_1^0 \\ y_2(D_n,F_n;0) - y_2^0 \end{bmatrix} . \tag{19}$$

Neglecting the second order terms in (16), we evaluate D_0 and F_0 as

$$D_0 = \zeta_2/y_2^0 \quad , \tag{20a}$$

$$F_0 = [y_1^0 - \zeta_1/D_0]\, D_0^\Gamma \quad , \tag{20b}$$

which are used as initial value in applying equation (19).

In Figure 1, we show the result of the calculation of y_1 using approximation

INSERT FIGURE 1

developed here. The curve is compared with the exact solution for the differential equation obtained using the Runge–Kutta (RK) method. The parameters used here are $t_\delta = 10$, $n = 1000$, $F_0 = 0.5$, $y_1(0) = 0.5$, $y_2(0) = 0.5$, $\alpha = 1$, $\beta = \gamma = 10$. We see that for times longer than 3, the approximation is good. The difference between the RK method and the approximation is in general small.

Figure 2 show y_1 for changing the parameter $\beta = \gamma = 1$. We see that the approximation result is poorer in all range of time.

INSERT FIGURE 2

In Figure 3, we show the result of the calculation y_2. The approximation is good fortimes longer than 3 and with $\beta = \gamma = 10$. For small times the approximation show

INSERT FIGURE 3

faster decay than the RK result.

In Figure 4, we show the result for y_2 $\beta = \gamma = 1$. The approximation method is far apart from the RK method. In the present case the approximation introduced a

INSERT FIGURE 4

dislocation of the origin of the reaction. This introduce an scale translation, givin the maximum for $t > 0$. In reality this maximum is expected to be at $t = 0$ in exact solution, and the time translation is attributed to the scale change from the approximation.

In Figure 5 we show the results for y_3. We see that the present approximation is

INSERT FIGURE 5

good for times longer than 3 using $\beta = \gamma = 10$. The y_3 raises from zero to a maximum and then decays faster or slowly accordingly to the kinetic processes involved. The RK method results are at shorter times and bigger values.

In Figure 6, we show that for $\beta = \gamma = 1$, the approximation gives poorer results in

INSERT FIGURE 6

all range of time. Also, we see that the maximum of RK is known smaller than the approximation results.

IV. CONCLUSIONS

For times long enough the solution is mainly dependent of ζ_2, because ζ_1 decrease fastly. In this case we see that for $\alpha \ll \gamma, \beta$, $r \sim \alpha \beta/\sqrt{2}\, \gamma F_0$. Thus y_1 and y_2 show the same for a constant relation $\alpha \beta/\gamma$. Thus for a fixed value α, we obtain the same curve for a constant relation β/γ. We reported this behavior in a previous work [16].

The approximation for the solution of the kinetic differential equations leave to smaller or bigger values of solution, as compared to the "exact" numerical solution. The results, although β/γ is constant, becames worst for bigger absolute values of β and γ.

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FIGURE CAPTIONS

Figure 1. Approximate (– – –) and exact values (RK method; ——) of y_1 for $\alpha = 1$, $\beta = \gamma = 10$.

Figure 2. Approximate (– – –) and exact values (RK method; ——) of y_1 for $\alpha = 1$, $\beta = \gamma = 1$.

Figure 3. Approximate (– – –) and exact values (RK method; ——) of y_2 for $\alpha = 1$, $\beta = \gamma = 10$.

Figure 4. Approximate (– – –) and exact values (RK method; ——) of y_2 for $\alpha = 1$, $\beta = \gamma = 1$.

Figure 5. Approximate (– – –) and exact values (RK method; ——) of y_3 for $\alpha = 1$, $\beta = \gamma = 10$.

Figure 6. Approximate (– – –) and exact values (RK method; ——) of y_3 for $\alpha = 1$, $\beta = \gamma = 1$.

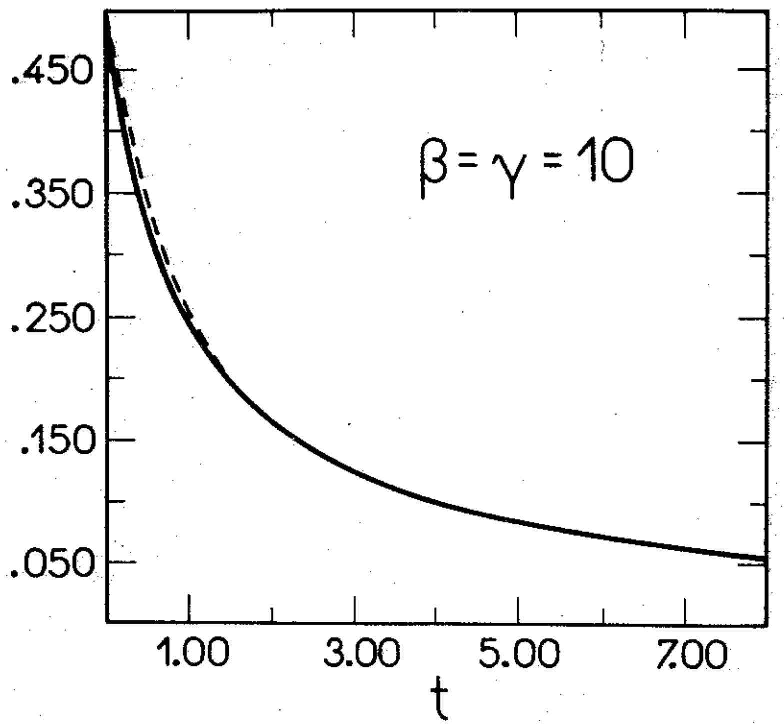


FIG. 1

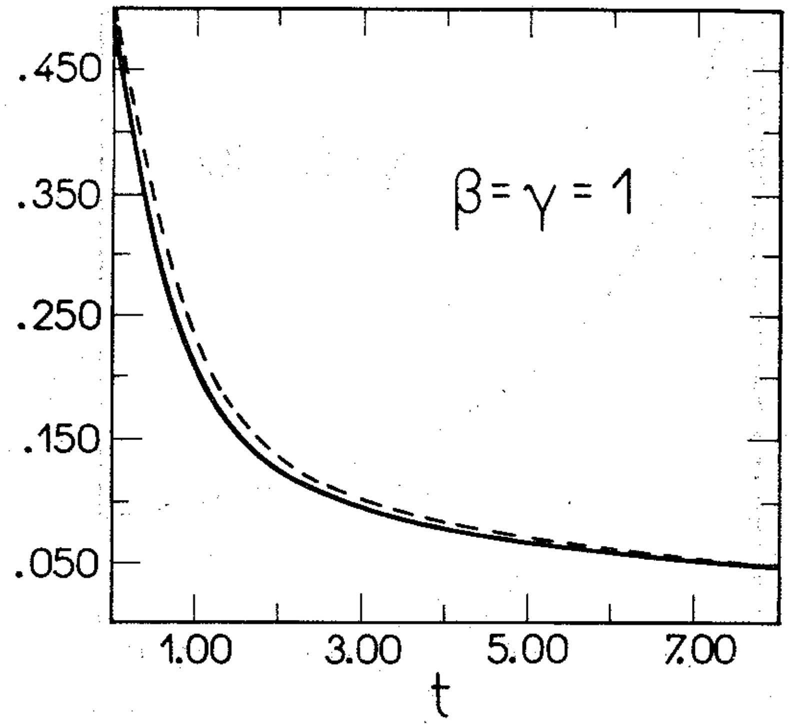
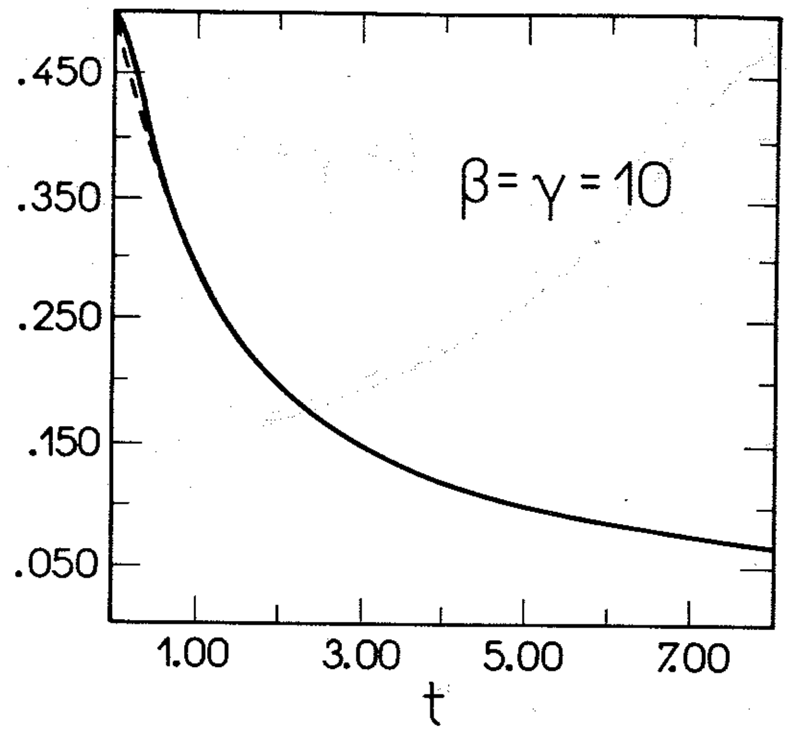

.450
.350
.250
.150
.050
β = γ = 1
1.00
3.00
5.00
7.00
t

FIG. 2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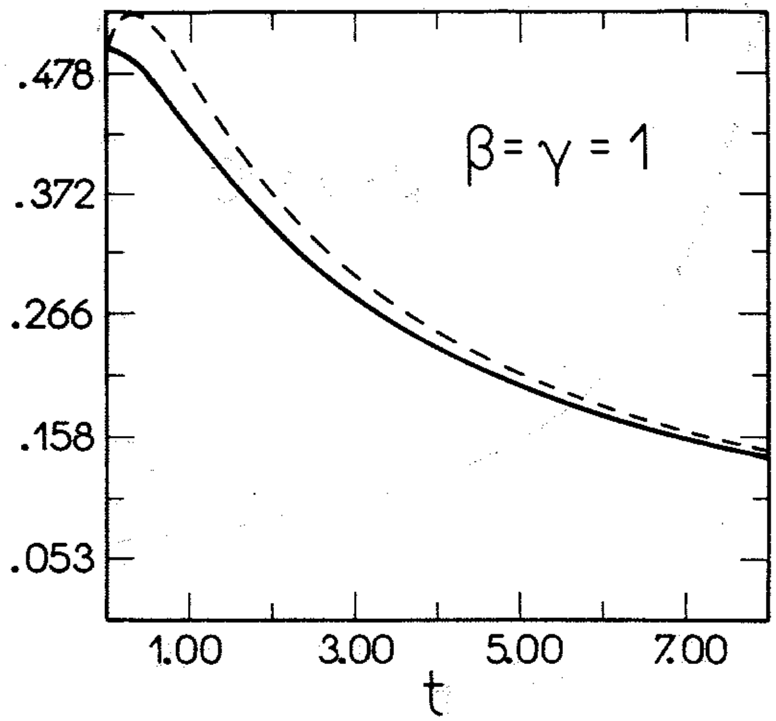
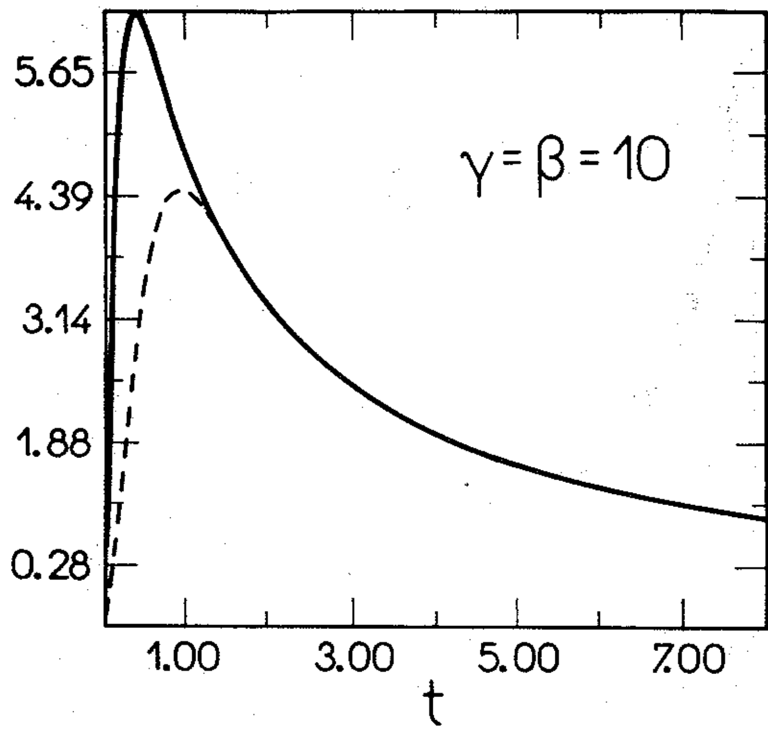
.350
.250
.150
.050
β = γ = 10
1.00
3.00
5.00
7.00
t

FIG. 3



.478
.372
.266
.158
.053
β = γ = 1
1.00
3.00
5.00
7.00
t

FIG. 4



5.65
4.39
3.14
1.88
0.28
γ = β = 10
1.00
3.00
5.00
7.00
t

FIG. 5

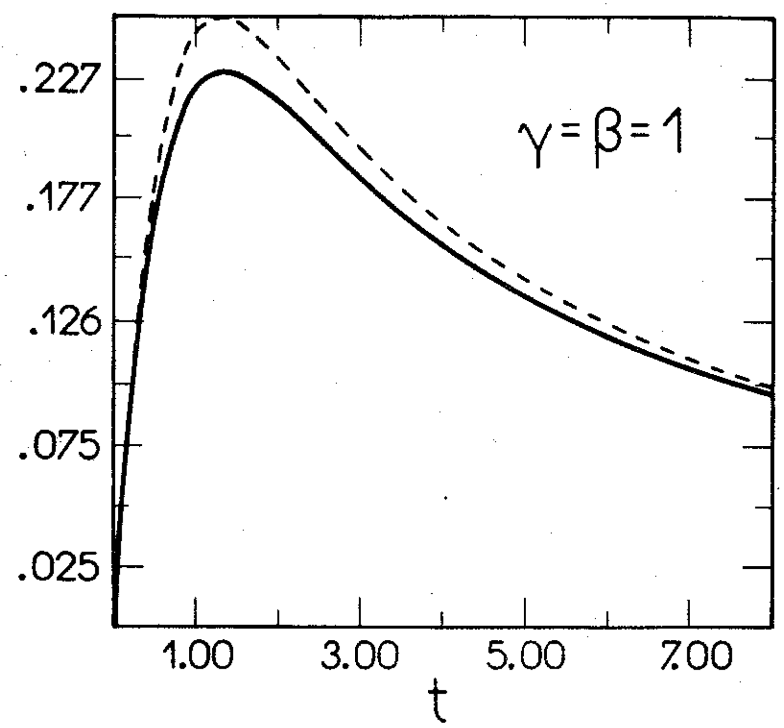


FIG. 6